

4-Nitrosodiphenylamine
156-10-5 | DTXSID1021031

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 10.3

Global applicability domain: Inside

Local applicability domain index: 4.26e-01

Confidence level: 5.84e-01

Nearest Neighbors from the Training Set

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Benzothiazole

Measured: 7.59

Predicted: 6.05

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N,N-Diethylaniline

Measured: 102

Predicted: 12.8

[Image not found](#)

N-Ethylaniline

Measured: 12.9

Predicted: 5.70

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Isophorone

Measured: 2.00

Predicted: 3.19